

Cyclopropanecarboxylic acid, 1-((4-chlorophenyl)sulfonyl)-, methyl ester
145348-22-7 | DTXSID60162991

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1.35

Global applicability domain: Inside

Local applicability domain index: 3.88e-01

Confidence level: 7.08e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Tris(2-chloroethyl) phosphate</div> <div>Measured: 1.29</div> <div>Predicted: 1.66</div>	<div>Image not found</div> <div>Dichlorvos</div> <div>Measured: 5.01e-01</div> <div>Predicted: 6.47e-01</div>	<div>Image not found</div> <div>Tris(2-chloroisopropyl)phosphate</div> <div>Measured: 7.94</div> <div>Predicted: 6.64</div>
<div>Image not found</div> <div>Triethyl phosphate</div> <div>Measured: 1.29</div> <div>Predicted: 1.38</div>	<div>Image not found</div> <div>Triallyl phosphate</div> <div>Measured: 1.20</div> <div>Predicted: 1.41</div>	